

UNIVERSITY OF WISCONSIN  
THEORETICAL CHEMISTRY INSTITUTE

TYPE OF REPORT: SEMI-ANNUAL PROGRESS REPORT to  
National Aeronautics and Space  
Administration (Theoretical  
Chemistry Institute Portion)

NUMBER OF REPORT: FIFTEEN (15)

PERIOD REPORT COVERS: 1 July 1969 through 31 December 1969

GRANT NUMBER: NGL 50-002-001

DATE: 31 December 1969

SIGNATURE:

  
\_\_\_\_\_  
Joseph O. Hirschfelder  
Principal Investigator

**CASE FILE  
COPY**

17 3245  
7203

## NASA SEMI-ANNUAL PROGRESS REPORT

The University of Wisconsin Theoretical Chemistry Institute is an integral part of the Department of Chemistry and has excellent working arrangements with the Physics, Mathematics, Computer Sciences and various Engineering Departments. Most of the permanent staff members hold joint appointments with these departments. In addition to their research, these staff members carry normal teaching loads and take their teaching responsibilities very seriously. In addition to graduate courses, they also teach undergraduate courses in elementary physical chemistry (laboratory as well as lecture), thermodynamics and reaction kinetics. We believe that our teaching program in theoretical chemistry is one of the best.

As a result of the NASA grant, the University of Wisconsin has been able to expand its theoretical chemistry faculty. We have noticed that the sharp improvement in the caliber of new graduate students and the quality of applicants of postdoctoral appointments at the Theoretical Chemistry Institute is continuing. In addition, a number of eminent professors are choosing to come to Wisconsin both for summer leaves and for sabbatical years in order to take advantage of the opportunities available at the Theoretical Chemistry Institute.

At the present time, we have 4 professors of chemistry, 1 professor of physics, 1 associate professor of chemistry, 1 visiting associate professor (part-time Mathematics Research Center), and 1 visiting associate professor of chemistry (on leave from M.I.T.). During this period, we have had 4 post-doctoral associates (3 NASA, 1 NSF supported). We have had 21 graduate students, including 7 research assistants (NASA supported),  $4\frac{1}{2}$  research assistants (NSF supported),  $4\frac{1}{2}$  teaching assistants (Univ. of

Wis. supported), 2 NSF Fellows, 2 NRC Fellows, and 1 self-supporting. These do not include the experimental students and post-doctoral associates working under Professors Bernstein, Cornwell, and Harriman. We have had a supervisor of our Theoretical Chemistry Institute computing center and 1 computer programmer.

At this time before reviewing the progress of the latest semi-annual period, we want to express our appreciation to the National Aeronautics and Space Administration (NASA) for providing the Theoretical Chemistry Institute with the opportunity for developing an excellent teaching and research program. The University of Wisconsin has also liberally contributed to the program of the Institute by paying the salaries for most of the permanent staff members, awarding teaching assistantships and graduate fellowships to many of our graduate students, and providing very excellent computing facilities.

We are very grateful to NASA for financing new facilities for the Theoretical Chemistry Institute. We now occupy all of the eighth floor and a part of the ninth floor of the new chemistry building. This provides us with ample space for all of our activities. We are especially pleased to have a very large specially constructed computing area with raised floor, separate power source, and separate air conditioning.

We are very sorry that NASA is not continuing the support of our research beyond fiscal year 1972. We feel strongly that Theoretical Chemistry will play an important role in the post-Apollo space program. We are indeed fortunate that the National Science Foundation is taking over the support of our research activities. However, we feel a very close attachment to NASA and hope that you will continue to regard us as part of your technical team.

RESEARCH INTERESTS OF THE THEORETICAL CHEMISTRY INSTITUTE STAFF

There is a wide range of research at the Theoretical Chemistry Institute. Saul T. Epstein and J. O. Hirschfelder are currently working on molecular and intermolecular quantum mechanics problems. C. F. Curtiss is concerned with the theory of statistical mechanics and transport properties. Richard B. Bernstein and C. F. Curtiss are interested in molecular beams and scattering theory. John E. Harriman is working on electron-spin resonance and quantum mechanical density matrices. C. Daniel Cornwell is working on microwave pressure broadening and other types of problems in molecular spectroscopy. The following is a summary of the detailed research interests of each of the staff members.

PERMANENT STAFFR. B. Bernstein

The research is in the area of molecular scattering, with the mainly experimental part of the program receiving support from NSF and the theoretical-computational part from NASA. The latter work is summarized below. Those members of the group involved in NASA-supported research for the period of this report are: Dr. M. T. Marron (whose report appears separately), Mr. R. J. LeRoy (a N.R.C. Fellow) and Mr. R. A. LaBudde.

Since the last progress report Dr. J. T. Muckerman has left for Brookhaven National Laboratory. From his Ph.D. Thesis, entitled "Rotational Compound State Resonances in Subthreshold Atom-Diatom Collisions", a further paper has been written, entitled "Complete Partial-Wave Treatment of Compound State (Rotational Excitation) Resonances in Subthreshold Scattering of an Atom by a Diatomic Molecule", J. Chem. Phys. (in press). This concludes our studies of the influence of these "internal excitation" resonances on the elastic scattering behavior of diatomic molecules, at least until experimental techniques in molecular beam scattering improve sufficiently to allow observation of the resonances.

A theme which has been recurrent in our work for many years is the dominant influence of the long-range interatomic forces upon the scattering behavior of atoms and molecules at thermal energies. In collaboration with Dr. A. S. Dickinson (former postdoctoral associate, now at the University of Stirling, Scotland) a paper has been written, entitled "Some Properties of Bound and Quasibound States for Various Interatomic



Potential Functions", Mol. Phys. (in press). Here semiclassical theory was employed to investigate the number of bound and quasibound states of diatomic molecules as a function of  $J$ , for various model potentials. The loss of vibrational levels with increasing  $J$  and the number of quasibound states (as well as their vibrational and rotational splittings) were found to depend mainly upon the long-range part of the interatomic potential. In a related research with R. J. LeRoy, an analysis was developed to use the vibrational spacings of the higher levels as a means of estimating the long-range internuclear potential function. As an important by-product of this work, an improved extrapolation technique was developed which supersedes the Birge-Sponer method for obtaining the dissociation energy of diatomic molecules. The first paper, describing the methodology, has been written (Report WIS-TCI-362); a second one, dealing with the practical applications, is in preparation. The connection between diatomic spectroscopy and atom-atom scattering has long been of interest to the group; this represents our concluding effort in this direction.

In the field of inelastic scattering, a paper has been written in collaboration with former postdoctoral associate Dr. W. A. Lester, Jr. (now at IBM, San Jose) entitled "Statistical Analysis of Transition Probability Matrices in the Strong Coupled Rotational Excitation Problem", J. Chem. Phys. (in press). Further research on the statistical approach is in progress; a joint manuscript, coauthored with Professor R. D. Levine (Hebrew University) is in preparation. A collaborative study has been initiated with Professor Curtiss and Dr. M. D. Pattengill to consider in detail the relationship between earlier approximation methods in rotational excitation theory (such as the time-dependent "sudden"

approximation) and a new formulation of the exact treatment recently developed by Curtiss which promises to be computationally feasible.

In the field of reactive scattering, R. A. LaBudde has been developing improved techniques for classical trajectory analysis of atom-diatom exchange reactions. Assuming a given potential energy surface, the classical equations of motion now may be efficiently solved, and the results of many suitably chosen trajectory computations combined to yield differential reactive scattering cross sections suitable for comparison with experiment. An optimum iterative program is sought which would lead to an improved potential surface. The question remains whether such classical treatments can ever be expected to explain quantitatively details of the product angular and recoil velocity distributions such as are now becoming available from our experimental studies. Further work in this direction is needed to ascertain the usefulness of this classical approach to reactive scattering.

In collaboration with the University of Toronto group a brief Communication has been written dealing with an application of the principle of microscopic reversibility (symmetry of the S-matrix) to some recent infrared chemiluminescence data. It is entitled: "Rates of the Endothermic Reactions  $\text{HCl} + \text{X}$  ( $\text{X} \equiv \text{I}, \text{Cl}$ ) as a Function of Reagent Vibration, Rotation and Translation", by K. G. Anlauf (now a postdoctoral here), D. H. Maylotte, J. C. Polanyi and R. B. Bernstein, J. Chem. Phys. (in press).

As an outgrowth of this work, Visiting Associate Professor J. L. Kinsey (on leave from M.I.T. as a Guggenheim Fellow) has undertaken a general consideration of the implications of microreversibility in



chemical reaction dynamics, which should lead to relationships of wide applicability. It should be noted that his presence here has appreciably enhanced the tone of our research group in both experimental and theoretical areas and is very much appreciated.

C. F. Curtiss

We have continued our study of transport phenomena in gases. In particular, we have continued the study of the effects of rotational degrees of freedom of molecules and also the effects of density on the transport coefficients.

The study of the effects of rotational degrees of freedom has led to an extensive study of the quantum mechanical theory of molecular scattering and a series of papers on this subject. The tenth paper in this series has recently been published and the eleventh has been accepted for publication. This series of papers, particularly the eighth paper, leads to a reformulation of the scattering integral equations. In the eleventh paper of the series, the reformulation is carried forward to a form more amenable to computation.

The development of the scattering theory referred to above leads largely to expressions for the degeneracy averaged cross sections. L. Hunter has extended the development to obtain general expressions for the detailed cross sections. He has also used the distorted wave approximation to obtain explicit expressions. The resulting expressions are consistent with the expressions we previously developed, in the tenth paper of the series, using the linearized sudden approximation.

We are now beginning to incorporate the results of the scattering theory into the kinetic theory expressions for the transport coefficients.

The scattering theory leads to expressions for the cross sections in terms of a generalized phase shift,  $H(\bar{\ell} S_a S_b)$ . When these expressions for the cross sections are used in the expressions for the transport coefficients some of the sums and integrations become "free" in the sense that they may, in principle, be carried out, in general, without a knowledge of the specific interaction. Our aim is to carry out as many of these operations as possible and express the transport coefficients in simpler forms without specifying the generalized phase shifts,  $H(\bar{\ell} S_a S_b)$ .

We have continued our study of density effects on the transport coefficients. David Bennett completed a thesis in which he extended to mixtures a treatment of the effects of collisional transfer and three body collisions which we had developed earlier. A paper based on this thesis has been published. Some time ago we developed a quantum mechanical treatment of the collisional transfer effects on the transport coefficients. Dennis Gibboney is developing a thesis in which the effects of three body collisions are introduced into the quantum mechanical formulation in a manner parallel to our previous classical development. He has completed the formal development and we are now considering the numerical evaluation of the various integrals which arise.

Saul T. Epstein

This past semester and presumably through the next year my research activities will revolve around and evolve from work on the proposed book "Perturbation Theory for Atoms and Molecules", in collaboration with Professors Byers Brown and Hirschfelder.

John E. Harriman

We have continued our studies of reduced density matrices and of systems with odd numbers of electrons. We are also concerned with relativistic quantum mechanics and magnetic interactions in atoms and molecules.

Continuing the work begun last year in collaboration with Dr. Janet Del Bene, we have formulated an approach to multiconfiguration calculations in density matrix terms. Although we have not yet found the reparametrization of the density matrix which we had hoped would simplify results, we do find that the formulation clarifies and simplifies the distinctions between purely combinational, symmetry, and truly dynamic aspects of the calculation. We are preparing to do some multiconfiguration calculations on open-shell systems using this formalism.

The concept of approximate N-representability, formulated with Mr. Jack Simons, has proved to be quite useful. We have defined a continuous measure of N-representability and have obtained expressions determining wave functions corresponding to density matrices that are as nearly N-representable as possible. A manuscript describing this work is in preparation.

Mr. James Tortorelli has calculated the isotropic and dipolar hyperfine interaction constants in  $H_2^+$ , as a function of internuclear distance, using the exact wave function. We expect to continue with similar calculations using approximate wave functions in  $H_2^+$  and  $H_3$  to gain an understanding of the effects of nuclear motion on calculated hyperfine interactions. Mr. Lloyd Holm has continued to work on programming for the approximate calculation of hyperfine interactions in larger molecules.

In the analysis of experimental ESR spectra to obtain data for comparison with the results of calculation, one is often confronted with difficulties in precise measurement because of line overlaps and of poor signal-to-noise ratio or other experimental problems. The possibility has now arisen in this Chemistry Department, as elsewhere, to digitize and record the experimental data in a form suitable for computer analysis. With Mr. Ken Brubaker, we have been developing programs to perform this analysis. We have been simulating spectra for analysis and hope to have the program operative by the time the digitized experimental spectra become available.

A large portion of my available time has been devoted to the preparation of a manuscript for a book on the theoretical foundations of electron spin resonance. I have been particularly concerned with the relativistic theory of the electron and its relationship to ordinary, non-relativistic quantum mechanics, and with surveying methods and examples of spin density calculation.

Joseph O. Hirschfelder

During the last six months I have concentrated on the mathematical formulation of perturbation theory for degenerate, almost degenerate and electron exchange problems. First I developed a formal treatment for the Rayleigh-Schrödinger theory for degenerate states where the degeneracy is resolved in an arbitrary order, then I shifted my attention to the partitioning techniques of Löwdin, Van Vleck, Kirtman, etc. Löwdin's treatment is very beautiful for infinite orders, but the Van Vleck-Kirtman approach is more useful for low-order treatments.



Dr. Phillip Certain and I have modified the Van Vleck-Kirtman approach to apply to electron exchange problems as well as to almost degenerate cases. This work will be very useful in determining intermolecular forces in intermediate separations where previous theory has been unsatisfactory. For electron exchange problems, the first order wave function is a sum of the usual polarization function plus an exchange function. We have concentrated our attention on the exchange function, which has very interesting properties. It introduces electron transfer terms into the molecular wave functions. We have determined the exchange function for the interaction of two hydrogen atoms numerically by making use of a variational principle together with a limited basis set. We have written three T.C.I. reports covering this work.

With Daniel Chipman (a graduate student) we have made a comparison between the Rayleigh-Schrödinger and the Primas Lie-algebra formulation of perturbation theory. We conclude that the Primas treatment is only useful for a very limited number of problems.

With Dr. Chris Wahl (at Argonne National Laboratory) my graduate student, Joseph Bowman, has been making Hartree-Fock self-consistent field calculations for the hydrogen molecule at intermediate to large separations using double precision calculations for high accuracy. The correlation energies were obtained to a high precision. At the equilibrium separation  $1.4 a_0$ , the correlation energy is about five times as large for the ground state as for the first excited state of the hydrogen molecule. At separations larger than  $8 a_0$ , these two correlation energies become equal. The gerade orbitals for the singlet and triplet states are very nearly the same at all separations. At small separations the ungerade orbital for the triplet state is much larger than that for

the singlet, but the two orbitals become comparable at large separations. At separations greater than  $5 a_0$ , there is no appreciable difference between the  $H_2^+$  and  $H_2$  orbitals. The extensive calculations were performed on the calculating machines at the Argonne National Laboratory.

With the graduate students, Mac Milleur and David Dion, I have made calculations of the transmission and reflection coefficients of wave packets on idealized potential energy surfaces using a method which was suggested by Dr. Peter Robinson (a visiting associate professor). The methods which we developed should be of considerable interest in the quantum-mechanical calculation of the rates of chemical reactions.

#### POSTDOCTORAL STAFF

##### Michael T. Marron

Work has continued on the classical hard sphere-loaded sphere model for reactive scattering which was discussed in the last (Fourteenth Semi-Annual) Progress Report. The equations of motion for the system have been solved analytically and the differential cross section, also found analytically, is a function of: the initial relative energy, vibrational exothermicity, initial rotational energy, the ratio of the initial and final reduced masses, and the distance of the load from the geometric center of the loaded sphere. The dependence of the differential cross section on these quantities is currently being examined in detail.

Work has begun on the formal development of a semiclassical impact parameter theory which treats the relative motion classically and the internal motion quantum mechanically. The trajectories determined by



the hard sphere-loaded sphere model will be used for the relative motion. Several conceptual difficulties arise regarding the quantum definition of internal states along classical trajectories. Provided these difficulties can be overcome, a practicable method results for determining the internal energy distribution of the reaction products. Such a theory would be extremely useful in photochemical studies and the development of chemical lasers.

In addition to the investigation of reactive scattering, two studies of the factors governing the binding energy of diatomic molecules have been completed. This work, based on the integral Hellmann-Feynman theorem, provides a new approach to a very old problem--what holds molecules together. The results of these studies are reported in two papers which have been accepted for publication in the Journal of Chemical Physics.

Carey M. Rosenthal

Since arriving in September, I have been working on an application of the perturbative treatment of exchange devised by Certain and Hirschfelder. The first order exchange equation for  $H_2$  and  $H_2^+$  is being studied and a transform of the solution has been obtained. (The  $H_2$  exchange equation can be reduced to a one electron problem and it is this problem which has been transformed and solved; the  $H_2^+$  exchange equation is of course also a one electron problem.) Work is progressing of the inversion of this transform.

John H. Young

Within the last six months I have initiated a theoretical investigation of energy conversion in biological systems in conjunction with Professor D. E. Green of the Institute of Enzyme Research, University of Wisconsin. The aim is to develop a detailed kinetic and thermodynamic model of oxidative phosphorylation and active transport in mitochondria. Through the analysis of a variety of experimental data we have determined that the energy-yielding redox reactions of the electron transport chain are coupled to an energy-requiring protein conformational transition. The relaxation of this metastable protein conformation is in turn coupled to the synthesis of adenosine triphosphate (ATP) or to the movement of ions across the inner mitochondrial membrane via a conformationally induced change in the electrochemical potential across the membrane.

## APPENDIX A

Summary of Research at the Theoretical Chemistry InstituteDuring the period 1 July 1969 through 31 December 1969

PERTURBATION THEORIES OF WEAK INTERMOLECULAR FORCES by Phillip Robinson  
 Certain (Ph.D. Thesis) (supported by NASA)

Report No. WIS-TCI-347

dated 16 July 1969

One article accepted for publication in Chem. Phys. Letters, and several  
 others in preparation.

ABSTRACT

This thesis is a contribution to the development of a workable exchange perturbation theory for intermolecular forces. It is divided into three parts. The first part develops a perturbation formalism for degenerate and almost degenerate energy states. The formalism is related to methods of Van Vleck, Kato, Bloch, Hirschfelder, Kirtman, and Löwdin and can have a greater range of validity than the Rayleigh-Schrödinger perturbation theory. The second part extends the formalism to exchange problems and leads to the Hirschfelder-Silbey perturbation theory. A method of solving the first order equation is developed which reduces the many electron equation to one and two electron equations. The third part applies four different perturbation formalisms for exchange forces to three model problems: the hydrogen molecule at internuclear separations  $R = 4, 6, 8 a_0$ ; a harmonic oscillator model of the hydrogen molecule ion; and the delta-function model of the hydrogen molecule ion.

COMPLETE PARTIAL WAVE TREATMENT OF COMPOUND STATE (ROTATIONAL EXCITATION)  
 RESONANCES IN SUBTHRESHOLD SCATTERING OF AN ATOM BY A DIATOMIC MOLECULE  
 by J. T. Muckerman and R. B. Bernstein (supported by NSF and NASA)

Report No. WIS-TCI-348

dated 25 July 1969

J. Chem. Phys. (January, 1970).

ABSTRACT

The present study deals with quantitative prediction of compound state resonance energies and widths in the elastic scattering of a diatomic molecule at energies below the threshold for rotational excitation. Previous work had been restricted to the weak interchannel coupling limit or to s-wave scattering only (but with no restriction on coupling strength). The adiabatic decoupling approximation, adequate to describe the s-wave resonance phenomenon, requires generalization to be applicable to higher partial waves. This extension is carried out and calculations yield good agreement with exact (close-coupled) results. It is then used in the numerical solution of the complete subthreshold resonance problem for an example involving moderately strong coupling, for which other approximate methods are inadequate. The present decoupling approximation, which yields accurate energies and semi-quantitative lifetimes of the compound states, leads also to a spectroscopic correlation scheme, i.e., an indexing of the spectrum of resonances.

MOLECULAR COLLISIONS, XI by C. F. Curtiss (supported by NASA)

Report No. WIS-TCI-349

dated 21 July 1969

Accepted for publication in J. Chem. Phys.

ABSTRACT

The development of Paper VIII of the series is continued to obtain equations and expressions suitable for the numerical evaluation of the cross sections for rotational excitation in collisions of rigid diatomic molecules interacting through an arbitrary soft potential. Explicit equations which describe collisions between an atom and a diatomic molecule are also given. An approximate solution of the equations is discussed.

CROSSED BEAM MEASUREMENTS OF DIFFERENTIAL ELASTIC SCATTERING OF Ar BY  $N_2$  : RAINBOW EFFECT AND INTERMOLECULAR POTENTIAL WELL DEPTH  
by Robert W. Bickes, Jr. and Richard B. Bernstein (supported by NSF and NASA)

Report No. WIS-TCI-350X

dated 25 July 1969

Chem. Phys. Letters 4, 111 (1969).

#### ABSTRACT

Differential cross section measurements for scattering of Ar (nozzle beam) by  $N_2$  [ $\theta$  (c.m.) range:  $3.8^\circ$  to  $45^\circ$ ] show classical low angle behavior ( $\sim \theta^{-7/3}$ ) and the rainbow effect at wider angles. The deduced well depth [for a L.-J. (12,6) potential] is  $1.4_0 \times 10^{-14}$  erg ( $\pm 10\%$ ).

THE EXCHANGE FUNCTION W FOR  $H_2$  AND  $H_2^+$   
by Phillip R. Certain and Joseph O. Hirschfelder (supported by NASA and PRC's NSF Fellowship)

Report No. WIS-TCI-351

dated 12 August 1969

This manuscript will not be submitted for publication.

#### ABSTRACT

In the new partitioning perturbation formalism for electron exchange problems, the exchange function W plays an important role. For  $H_2$  and  $H_2^+$  the W is determined variationally in terms of a 14 term Slater orbital basis set. Tables are given for expressing W at 14 values of the internuclear separation ranging from  $R=1a_0$  to  $20a_0$ .

SPECTROSCOPIC REASSIGNMENT AND GROUND STATE DISSOCIATION ENERGY OF MOLECULAR IODINE

by Robert J. LeRoy (supported by NSF and NASA)

Report No. WIS-TCI-331 Revised\*

dated 13 August 1969

Accepted for publication in J. Chem. Phys.

#### ABSTRACT

Re-analyzing some early band head data for  $I_2(B\ 0_u^+(^3\pi))$ , an improved value of the ground state dissociation energy is found to be



$D_0 = 12429(+4) \text{ cm}^{-1}$ , differing significantly from the previously accepted value of R. D. Verma ( $12452.5(+1.5) \text{ cm}^{-1}$ ). This result implies that the final state of one of the UV resonance series reported by R. D. Verma must have a rotationless potential maximum some  $25(+5) \text{ cm}^{-1}$  high. It is further shown that the original electronic assignment of this state as ground state  $X O_g^+(^1\Sigma)$  is implausible. A reassignment as  $O_g^+(^3\Pi)$  is proposed and the nature of the  $O_g^+(^3\Pi)$  potential is considered.

#### PREDICTED SPECTRUM OF SUBTHRESHOLD ROTATIONAL COMPOUND STATE

RESONANCES:  $p\text{-H}_2\text{-Xe}$  and  $o\text{-D}_2\text{-Xe}$

by J. T. Muckerman and R. B. Bernstein (supported by NSF and NASA)

Report No. WIS-TGI-352 \*

dated 15 August 1969

Chem. Phys. Letters 4, 183 (1969).

#### ABSTRACT

Rotational compound state resonances in subthreshold atom-diatom scattering are calculated for  $p\text{-H}_2\text{-Xe}$  and  $o\text{-D}_2\text{-Xe}$  via a complete partial-wave treatment yielding resonance energies and widths. The predicted resonance spectra might be observable in high resolution molecular beam scattering experiments.

COMPARISON OF PRIMAS AND RAYLEIGH-SCHRÖDINGER PERTURBATION THEORIES  
by D. M. Chipman and J. O. Hirschfelder (supported by NASA)

Report No. WIS-TGI-353

dated 18 August 1969

This manuscript will not be submitted for publication as of now.

#### ABSTRACT

The Primas and Rayleigh-Schrödinger formulations of perturbation theory are compared in considerable detail. The Primas approach appears useful only in special cases where the operators involved form a Lie algebra with a small number of elements. For Hamiltonians with degenerate energy levels or for many body systems, the Primas formalism does not appear practical.



## INTERACTION DIPOLE BETWEEN RARE-GAS ATOMS

by W. Byers Brown and D. M. Whisnant (supported by NSF and NASA)

Report No. WIS-TCI-355

dated 27 August 1969

This manuscript will be submitted for publication.

ABSTRACT

A new formula is derived for the coefficient  $D_7$  of the leading term in  $R^{-7}$  for the electric dipole moment of two atoms in S-states at a large distance  $R$  apart. An approximation is proposed which leads to a simple formula for  $D_7$  involving mainly accessible atomic properties; the approximation is checked for scaled hydrogen atoms and is accurate to about one per cent. Rough values of  $D_7$  are calculated for the rare-gas diatoms which indicate that the dispersion dipoles are of the opposite sign from the overlap dipoles calculated by Matcha and Nesbet (1967), and can be of the same order of magnitude. A simple perturbation approach to the overlap dipole is proposed.

## ROTATIONAL COMPOUND STATE RESONANCES IN SUBTHRESHOLD ATOM-DIATOM COLLISIONS (Ph.D. Thesis)

by James Terry Muckerman (supported by NSF and NASA)

Report No. WIS-TCI-356

dated 28 August 1969

Most of this manuscript has been published or is now in press.

ABSTRACT

Resonance behavior in subthreshold scattering of atoms by rigid diatomic molecules is demonstrated by exact (close-coupled) calculations involving the solution of the Schrödinger equations with closed channels included in the basis set. These resonances arise from virtual (rotational) inelastic processes resulting in the formation of temporarily excited diatom-atom bound states, and are, in principle, observable as rapid disturbances in the energy dependence of the integral elastic scattering cross section.

Each "isolated" resonance is characterized by an energy and width by fitting the exactly calculated phase shifts to a Breit-Wigner resonance form. Decoupling approximations, which treat the interchannel coupling in a perturbative manner, are tested by comparison with the exact numerical results. The "adiabatic" decoupling approximation introduced by R. D. Levine is found to predict quite accurately the resonance energies (as well as the non-resonant phase shifts) for all partial waves. This decoupling procedure is extended to allow the prediction of resonance widths. The results are found to agree with the exact resonance widths for s-wave collisions (a two-state problem), but are much less accurate for higher partial waves (in general, a four-state problem). The approximation for the non-s-wave resonance widths is considerably improved by the use of a renormalization procedure.

The complete subthreshold rotational compound state resonance "spectra" for several physically realistic model systems ( $p\text{-H}_2\text{-He}$ ,  $p\text{-H}_2\text{-Xe}$ , and  $o\text{-D}_2\text{-Xe}$ ) are calculated using the extended adiabatic decoupling procedure. Results are discussed in terms of the possibility of observing such resonance behavior in future molecular beam scattering experiments.

CALCULATED TOTAL ELASTIC SCATTERING CROSS SECTIONS FOR  $\text{H}(1s) + \text{H}(1s)$   
AT COLLISION ENERGIES BELOW 1eV by Michael E. Gersh and Richard B.  
Bernstein (supported by NSF and NASA)

Report No. WIS-TCI-357

dated 29 August 1969

Chem. Phys. Letters 4, 221 (1969).

ABSTRACT

Exact computations of the elastic scattering cross sections for atomic hydrogen, based on the best local  $^1\sum_g^+$  and  $^3\sum_u^+$  potentials, provide an accurate, essentially ab initio prediction of glory and resonance behavior to be expected in H(1S) beam scattering experiments.

A VERSATILE MOLECULAR BEAM APPARATUS UTILIZING ELECTRON IONIZATION DETECTION: OBSERVATION OF THE RAINBOW EFFECT FOR ARGON-NITROGEN by Robert William Pickes, Jr. (Ph.D. Thesis) (supported by NSF and NASA)

Report No. WIS-TCI-358X

dated 15 September 1969

This manuscript will not be published in its present form.

(EXPERIMENTAL ONLY)

CALCULATIONS FOR A QUANTUM-MECHANICAL MODEL OF THE REACTIVE SCATTERING OF THREE ATOMS ON A LINE by David R. Dion, Mac B. Milleur, and Joseph O. Hirschfelder (supported by NSF and NASA)

Report No. WIS-TCI-359

dated 8 October 1969

Accepted for publication in J. Chem. Phys.

ABSTRACT

In a companion paper, P. D. Robinson shows that the basis set which Halburdt and Hirschfelder used to obtain the transmission and reflection coefficients for a quantum mechanical model of reactive scattering of three atoms in a line was incomplete for a set of resonance energies. In the present paper, using Robinson's complete basis set, agreement is obtained with Tang, Kleinman, and Karplus's estimate of the transmission coefficient for  $E(8\mu^2/h^2) = 2$ . It is found that the "point matching" method of solution does not converge as rapidly as the truncated Fourier series. Graphs of the flux and particle density are given.

ON ENERGY BOUNDS DERIVED FROM THE CONJUGATE EIGENVALUE PROBLEM  
 by Peter L. Robinson and Saul T. Epstein (supported by NSF, NASA and Math  
 Research Center, U.S. Army)  
 Report No. WIS-TCI-360 dated 13 October 1969

This manuscript has been submitted for publication.

#### ABSTRACT

An upper bound for  $E_0$ , which has been derived from the conjugate eigenvalue problem by Hall, is discussed. It is emphasized that the bound is only guaranteed when  $V$  is negative-definite. An alternative bound is presented which is free from this restriction, and the underlying iterative procedure is given. Hall's result is generalized to admit internuclear distances, and the theory is illustrated by a one-dimensional system with delta-function potentials. Some disadvantages of the approach are mentioned.

THE VARIATIONAL METHOD IV - LOWER BOUNDS FOR THE ENERGY by Saul T. Epstein  
 (supported by NASA)

Report No. WIS-TCI-361 dated 21 October 1969  
 This manuscript will not be submitted for publication.

DISSOCIATION ENERGY AND LONG-RANGE POTENTIAL OF DIATOMIC MOLECULES FROM  
 VIBRATIONAL SPACINGS OF HIGHER LEVELS by Robert J. LeRoy and Richard B.  
 Bernstein (supported by NSF, NASA and RJL's NRC Scholarship)

Report No. WIS-TCI-362 dated 13 November 1969

This manuscript has been submitted for publication.

#### ABSTRACT

An expression is derived which relates the distribution of vibrational levels near the dissociation limit  $D$  of a given diatomic species to the nature of the long-range interatomic potential in the region where the latter may be approximated by  $D - C_n/R^n$ . Fitting experimental energies directly to this relationship yields values of  $D$ ,  $n$ , and  $C_n$ . This procedure requires a knowledge of the relative energies and relative



vibrational numbering for at least four rotationless levels lying near the dissociation limit; however, it requires no information on the rotational constants, or on the number and energies of the deeply bound levels.  $D$  can be evaluated with a much smaller uncertainty than heretofore obtainable from Birge-Sponer extrapolations. The formula predicts the energies of all vibrational levels lying above the highest one measured, with uncertainties no larger than that of the binding energy of the highest level. The validity of the method is tested with model potentials and its usefulness is demonstrated by application to the precise data of Douglas, Møller, and Stoicheff for the  $B^3\pi_{Ou}^+$  state of  $Cl_2$ .

INTEGRAL HELLMANN-FEYNMAN ANALYSIS OF THE BINDING ENERGY OF  $H_2$  AND  $LiH$  USING ATOMIC REFERENCE-STATES by Michael T. Marron (supported by NASA)

Report No. WIS-TCI-363

dated 4 November 1969

Accepted for publication in J. Chem. Phys.

#### ABSTRACT

The integral Hellmann-Feynman formula is applied to study the energy differences involved in the processes  $He \longrightarrow H_2 \longrightarrow H^-$  and  $Be \longrightarrow LiH \longrightarrow Li^-$ . The energy differences are computed using single determinant SCF wavefunctions to represent the states. The transition density is reduced to diagonal form by means of a corresponding orbital transformation and each term in the energy expressions for the  $Be \longrightarrow LiH \longrightarrow Li^-$  process is given a physical interpretation in terms of classical electrostatic concepts. A qualitative discussion is given which indicates a simple model might readily account for all factors contributing to the energy difference.

THE DISSOCIATION OF DIATOMIC MOLECULES FROM THE VIEWPOINT OF THE INTEGRAL HELLMANN-FEYNMAN FORMULA:  $H_2$ , LiH, and  $Li_2$  by Michael T. Marron (supported by NASA and a research grant to The Johns Hopkins University from NIH)

Report No. WIS-TCI-364

dated 10 November 1969

Accepted for publication in J. Chem. Phys.

#### ABSTRACT

The integral Hellmann-Feynman formula is used to compute the dissociation energies of  $H_2$ , LiH, and  $Li_2$ . The derivation of the transition densities and the method of taking the limit of the transition densities as one of the nuclei is removed to infinity, is discussed. The expression for the dissociation energy of LiH is examined in detail. While the results (except for  $H_2$ ) are inaccurate, it is argued that the essential characteristics of the transition density are correctly determined and that the method provides a basis for the physical interpretation of the factors which contribute to the dissociation energy.

NEW PARTITIONING PERTURBATION THEORY: I. GENERAL FORMALISMS by Phillip R. Certain and Joseph O. Hirschfelder (supported by FRC's NSF Fellowship and NASA)

Report No. WIS-TCI-365

dated 20 November 1969

This manuscript has been submitted for publication.

#### ABSTRACT

By the use of partitioning techniques, a general formalism is developed for considering degenerate, almost degenerate, and electron exchange perturbation problems. In effect, we generalize the Van Vleck-Kirtman approach to arbitrary orders and arbitrary normalization and obtain three types of approximations: In the Modified Kirtman treatment the functions through the N-th order are fully normalized and the energy is obtained as the roots of the secular equation. The DE-FOP-VIM



approximation is the same except that the normalization of the functions is energy optimized. The Kirtman approximation uses the same functions as the Modified Kirtman but the energy is obtained as the roots of a much simpler secular equation which results from a factorization of the original secular equation (except for terms of order  $2N+2$ ). The Kirtman energies are not upper bounds. LBwdin's formalism is equivalent to the Modified Kirtman with the exception that LBwdin uses intermediate normalization. Electron exchange problems are considered more explicitly in a companion paper with the use of symmetry considerations.

NEW PARTITIONING PERTURBATION THEORY: II. EXAMPLE OF ALMOST DEGENERACY  
by Phillip R. Certain, David R. Dion, and Joseph O. Hirschfelder  
(supported by PRC's NSF Fellowship and NASA)

Report No. WIS-TCI-366

dated 24 November 1969

This manuscript has been submitted for publication.

#### ABSTRACT

A system of two coupled simple harmonic oscillators where many of the energy levels are almost degenerate doublets serves as an excellent "guinea pig" for testing any perturbation techniques including the Modified Kirtman, Kirtman, and DE-FOP-VIM treatments discussed by Certain and Hirschfelder in a companion paper. These methods are compared with the "usual" approach to almost degenerate problems which makes the zeroth order energies of the doublet pair degenerate by a suitable choice of the zeroth order hamiltonian. In addition, four types of Rayleigh-Schrödinger expansions are considered. The best values of the energy are given by the Kirtman treatment. However, the DE-FOP-VIM and the Modified Kirtman procedures give values almost as good, and have the added advantage that they give upper bounds to the energy of the states which are considered.

NEW PARTITIONING PERTURBATION THEORY: III. APPLICATIONS TO ELECTRON EXCHANGE by Phillip R. Certain and Joseph O. Hirschfelder  
(supported by PKC's NSF Fellowship and NASA)

Report No. WIS-TCI-367 dated 28 November 1969  
This manuscript has been submitted for publication.

#### ABSTRACT

A new partitioning perturbation technique provides a rigorous derivation and generalization of the Hirschfelder-Silbey formalism for treating electron exchange problems. A new method of solving the first order perturbation equation is introduced. The first order wave function is the sum of the polarization function which describes van der Waals correlations and an exchange function which introduces ionic terms. The exchange function is determined variationally for both the ground state  $H + H^+$  and  $H + H$  interactions. In the many electron case, the first order equation reduces to a set of one and two electron equations.

NOTE ON THE SIMPLE COLLISION THEORY OF REACTIVE HARD SPHERES by Michael T. Marron (supported by NASA)

Report No. WIS-TCI-368 dated 21 November 1969  
This manuscript has been submitted for publication.

A TRANSFORM FOR TREATING A WIDE CLASS OF PERTURBATION PROBLEMS, WITH APPLICATION TO THE EXCHANGE EQUATIONS FOR  $H_2^+$  AND  $H_2$  by Carey M. Rosenthal (supported by NASA)

Report No. WIS-TCI-371 dated 24 November 1969  
This manuscript will be submitted for publication.

#### ABSTRACT

A transform is introduced to solve the  $H_2^+$  and  $H_2$  exchange functions of Certain and Hirschfelder. The solution obtained for  $H_2^+$  is compared numerically with a variational function. The properties of this transform are derived and its applicability to other perturbation problems is discussed.

HARTREE-FOCK CALCULATIONS FOR THE GROUND AND FIRST EXCITED STATES OF  $H_2$  by Joseph D. Bowman, Jr., Arnold C. Wahl, and Joseph O. Hirschfelder (supported by NSF and NASA)

Report No. WIS-TGI-373 dated 15 December 1969  
This manuscript will be submitted for publication.

#### ABSTRACT

The Hartree-Fock energy and orbitals are calculated with high precision for both the ground state ( $^1\Sigma_g^+$ ) and the first excited state ( $^3\Sigma_u^+$ ) of  $H_2$  for separations ranging from the United Atom to  $10a_0$ . The  $\sigma_g$  orbital obtained from the  $^1\Sigma_g^+$  is almost the same as that from the  $^3\Sigma_u^+$  for all separations. However when  $R > 5a_0$ , the  $\sigma_u$  from the  $^3\Sigma_u^+$  is larger than that from the  $^1\Sigma_g^+$ . The correlation energy ( $E_{HF} - E$ ) is 4 times larger for the  $^1\Sigma_g^+$  than for the  $^3\Sigma_u^+$  at the equilibrium separation,  $1.4a_0$ . For separations greater than  $8a_0$ , the two correlation energies become equal.

DIRECT CALCULATION OF SECOND-ORDER DENSITY MATRIX I. THEORY OF THE GREEN'S FUNCTION TECHNIQUE by Jack Simons (supported by JS' NSF Fellowship and NASA)

Report No. WIS-TGI-374\* dated 16 December 1969  
This manuscript will be submitted for publication.

#### ABSTRACT

We present a method for directly determining the second-order density matrix of a system of particles with pairwise additive interactions. The result is obtained as a contour integral involving the two-particle Green's function. The random phase approximation is made and the evaluation of the Green's function is reduced to a simple matrix problem. An outline of the computational method is presented, and possible applications are discussed.

APPRAISAL OF AN ITERATIVE METHOD FOR BOUND STATES by Peter D. Robinson ,  
Tony T. Warnock and Norman Anderson (supported by NSF and NASA)

Report No. WIS-TOL-375\*

dated 18 December 1969

This manuscript will be submitted for publication.

# ABSTRACT

An iterative method for determining bound-state eigenvalues and properties of the radial Schrödinger equation is appraised. The method stems from iterating the integral equation

$$\Psi = \mu(T + \frac{1}{2}V)^{-1}(-V\Psi)$$

when  $T$  and  $V$  are the kinetic and potential energy operators. The basic theory is briefly reviewed, and calculations are performed for the Coulomb and Screened Coulomb potentials. The lowest three  $\mu$ -eigenvalues together with expected values of  $(\gamma r)^{-1}$ ,  $\gamma r$  and  $(\gamma r)^2$  are obtained from a single iterated eigenfunction sequence. Convergence is rapid for eigenvalues but slow for expected values. There is some sensitivity to the choice of numerical integration formula. Regarded as a numerical method, this approach may be most competitive for the determination of zero-energy potential-strength eigenvalues. Its disadvantages are listed.

Analytical improvements to eigenfunctions can be easier to obtain by iteration than by perturbation, and some success has been achieved. A simple example suggests that the rate of convergence of an iterated eigenfunction sequence is less than that of a related perturbation sequence unless the choice of starting function is bad.

\* - - -  
Copies of these reports are not available. Reprints of most of these articles will be available at a later date.



Additional Publications During the Period 1 July 1969 - 31 December 1969

"Rotational Excitation in Molecular Collisions: Exact (Two-State) Results Versus Variational (Decoupling) Computations" by R. D. Levine, M. Shapiro, J. T. Muckerman and R. R. Johnson, Chem. Phys. Letters 2, 545 (1968)

ERRATUM to J. Chem. Phys. 43, 1095 (1965): "Perturbation Treatment of the Ground State of  $H_2^+$ " by William D. Lyon, Robert L. Matcha, William A. Sanders, William J. Meath, and Joseph O. Hirschfelder, J. Chem. Phys. 51, 3151 (1969)

"Formal Rayleigh-Schrödinger Perturbation Theory for Both Degenerate and Non-degenerate Energy States" by Joseph O. Hirschfelder, Int. J. Quant. Chem. III, 731 (1969) (WIS-TCI-337)

"Sum Rules for Variational Wavefunctions" by A. Dalgarno and S. T. Epstein, J. Chem. Phys. 50, 2837 (1969)

"Reactive Scattering of K by HBr, DBr, in Crossed Molecular Beams: Angular and Velocity Distributions of KBr in Laboratory and c.m. Systems" by Keith T. Gillen, Glyde Riley and R. B. Bernstein, J. Chem. Phys. 50, 4019 (1969) (WIS-TCI-324X)

"Resonance Theory of Termolecular Recombination Kinetics:  $H + H + M \rightarrow H_2 + M$ " by Robert E. Roberts, R. B. Bernstein, and C. F. Curtiss, J. Chem. Phys. 50, 5163 (1969)

"Dipole Shielding Tensor" by Saul T. Epstein and Robert E. Johnson, J. Chem. Phys. 51, 188 (1969)

"First- and Second-Order Density Matrices of Symmetry-Projected Single-Determinant Wavefunctions" by Jack Simons and John E. Harriman, J. Chem. Phys. 51, 296 (1969) (WIS-TCI-334)

"Localized Orbital Description of the C-O Bond in Ketene" by Janet Del Bene, J. Chem. Phys. 51, 2290 (1969) (WIS-TCI-343)

"Molecular Collisions. X. Restricted-Distorted-Wave-Born and First-Order Sudden Approximations for Rotational Excitation of Diatomic Molecules" by R. W. Fenstermaker, C. F. Curtiss, and R. B. Bernstein, J. Chem. Phys. 51, 2439 (1969) (WIS-TCI-344)

"Density Effects on the Transport Coefficients of Gaseous Mixtures" by David E. Bennett III and C. F. Curtiss, J. Chem. Phys. 51, 2811 (1969)

"Potential Flows of Dilute Polymer Solutions by Kramer's Method" by R. Byron Bird, Millard W. Johnson, Jr. and Charles F. Curtiss, J. Chem. Phys. 51, 3023 (1969)

"A Statistical Derivation of the Hydrodynamic Equations of Change for a System of Ionized Molecules. I. General Equation of Change and the Maxwell Equations" by R. J. Beshinske and C. F. Curtiss, J. Stat. Phys. 1, 163 (1969)

"On the Use of Morse Eigenfunctions for the Variational Calculation of Bound States of Diatomic Molecules" by E. M. Greenawalt and A. S. Dickinson, J. Mol. Spec. 30, 427 (1969) (WIS-TCI-315)

"Simplistic Analysis of Reactive Scattering" by R. D. Levine and R. B. Bernstein, Israel J. Chem. 7, 315 (1969) (20th Farkas Memorial Symposium)

"N-Representability Problem: Conditions on Geminals" by Mary Beth Ruskai, Phys. Rev. 183, 129 (1969) (WIS-TCI-329)

-----

The following reports have not been included in Appendix A since they were supported by NSF only:

THE N-REPRESENTABILITY PROBLEM by Mary Beth Ruskai (Ph.D. Thesis), parts of this manuscript have been published (WIS-TCI-346)

SOLUTION OF THE HELMHOLTZ EQUATION ON A SQUARE FOR A REACTIVE SCATTERING MODEL by Peter D. Robinson, accepted for publication in J. Chem. Phys. (WIS-TCI-354)

MOLECULAR COLLISIONS, XII: GENERALIZED PHASE SHIFTS by C. F. Curtiss, submitted for publication in J. Chem. Phys. (WIS-TCI-370)



APPENDIX BUniversity of Wisconsin Theoretical Chemistry Institute Staff During  
the Period July 1, 1969 through December 31, 1969FACULTY

<u>Name</u>	<u>Title</u>
Joseph O. Hirschfelder	Professor of Chemistry; Director, Theoretical Chemistry Institute
C. F. Curtiss	Professor of Chemistry; Associate Director, Theoretical Chemistry Institute
Richard B. Bernstein	Professor of Chemistry
C. D. Cornwell	Professor of Chemistry
Saul T. Epstein	Professor of Physics
John E. Harriman	Associate Professor of Chemistry

VISITING PROFESSORS

James L. Kinsey	Visiting Associate Professor of Chemistry (Academic Year 1969-1970; on leave from M.I.T.; Guggenheim Fellow)
Peter D. Robinson	Visiting Associate Professor of Chemistry (7/69-12/69; part-time Mathematics Research Center; on leave from Department of Mathematics, University of York, England)

POSTDOCTORAL STAFF

Michael T. Marron Johns Hopkins University Ph.D. 1969	Project Associate
Merle D. Pattengill Univ. of California, Irvine Ph.D. 1969	Project Associate
Carey M. Rosenthal Harvard University Ph.D. 1969	Project Associate
John H. Young Univ. of California, Berkely Ph.D. 1966	Project Associate

COMPUTING STAFF

<u>Name</u>	<u>Title</u>
Wanda W. Giese	Project Specialist (Part-time: $\frac{1}{4}$ NSF, $\frac{1}{4}$ NASA supported)
Tony T. Warnock	Project Assistant (Part-time: $\frac{1}{4}$ NSF, $\frac{1}{4}$ NASA supported)

GRADUATE STUDENTS

Michael F. Barnsley	Research Assistant
Scott C. Bello	Teaching Assistant
Joseph D. Bowman	Research Assistant
Kenneth L. Brubaker	Research Assistant
Phillip R. Certain	NSF Fellow and Research Assistant (now Ph.D.)
Daniel M. Chipman	Research/Teaching Assistant
Albert C. Christoph	Teaching Assistant
David R. Dion	Research Assistant
Dennis A. Gibboney	Research Assistant
Russell D. Hageman	Research Assistant
Lloyd M. Holm	Research Assistant
Lawrence W. Hunter	NRC Fellow
Samuel E. Konkin	No support
Robert A. LaBudde	Research Assistant
Robert J. LeRoy	NRC Fellow
Mac B. Milleur	Research Assistant
James T. Muckerman	Research Assistant (now Ph.D.)
Richard D. Olmsted	Teaching Assistant
John P. Simons	NSF Fellow
James J. Tortorelli	Research Assistant
David M. Whisnant	Research Assistant

SECRETARIAL STAFF

<u>Name</u>	<u>Title</u>
Sheila E. Battle	Administrative Secretary II (½ NSF supported)
Maureen B. Hill	Typist III (½ NSF supported)
Gloria M. Lawton	Stenographer III (100% NASA supported)
Linda L. Stoltenberg	Stenographer II (½ NSF supported)

## APPENDIX C

University of Wisconsin Theoretical Chemistry Institute Short-TermVisitors During the Period July 1, 1969 through December 31, 1969

<u>NAME AND ADDRESS</u>	<u>PERIOD OF VISIT</u>	<u>LECTURES GIVEN</u>
Prof. W. Byers Brown Dept. of Chemistry University of Manchester Manchester, England	7/1-8/31/69	Panel Discussion on Alkali Metal Clusters  Perturbation Theory of Short Range Atomic Inter- actions. Part II
Prof. Clifton R. Blincoe Biochemistry Division University of Nevada Reno, Nevada	7/1-8/31/69	
Dr. Robert A. Sack Dept. of Mathematics University of Salford Salford, Lancs., England	7/22-26/69	A Simple Approach to Spherical Harmonics
Prof. F. A. Matsen Dept. of Chemistry University of Texas Austin, Texas	8/3-31/69	I. Chemistry Without Spin II. The Aggregate Theory of Polyelectronic Systems
Dr. Brian Sutcliffe Dept. of Chemistry University of York York, England	8/19-21/69	Molecular Calculations Not Making Fixed Nuclei Approximations
Prof. R. D. Levine Dept. of Chemistry The Hebrew University Jerusalem, Israel	8/25-28/69 9/23-25/69 10/27/69	Decoupling Approximations in Molecular Scattering Theory  Panel Discussion on Long-Lived Complexes in Molecular Scattering
Dr. Werner Kutzelnigg Theoretical Chemistry Group University of Göttingen 34 Göttingen Burgerstrasse 50a, Germany	9/25/69	A Novel Approach to the Calculation of Inter- molecular Forces with Application to the van der Waals Constant of Alkali Atom Pairs
Dr. Norman Bazley Advanced Studies Center Battelle Institute Geneva, Switzerland	10/16/69	Estimation of Expectation Values for Schrödinger Operators

Professor Howard Taylor  
Dept. of Chemistry  
Univ. of Southern California  
Los Angeles, California

10/27-28/69

Theoretical Interpretation  
of the Electron Scattering  
Spectrum of CO<sub>2</sub>

On the Many-Body Theory of  
the Elastic Scattering of  
Electrons from Atoms and  
Molecules